DAAB07-97-C-6005

HYDROGEN SUPPLY SYSTEM FOR SMALL PEM FUEL CELL STACKS

L. Staples and D. P. Bloomfield
Analytic Power Corp.
268 Summer Street
Boston, MA 02210

Final Technical Report

Period: October 1996 - July 1997

Approved for Public Release - Distribution is Unlimited

Prepared for
U.S. ARMY CECOM RD&E CENTER-SOUTH
ATTN: AMSEL-RD-C2-PD-E
10108 GRIDLEY RD., SUITE 1
FT. BELVOIR, VA 22060-5817

20011128 095

1. INTRODUCTION

This program was to determine how to employ thermolysis of chemical hydrides to produce low cost hydrogen for Soldier Power System (SPS) type fuel cells. Originally, the program was directed at the Digital Reactor concept. Early in the program, we determined that the digital reactor could not be made safe, light weight, or at low cost. We attempted to find an alternative to the digital reactor which, while still employing Beckert Dengel thermoloysis chemistry, could be made safe, light weight, and inexpensive. We failed in that attempt as well. This report documents the fundamental problems to be overcome in developing a chemical hydride based hydrogen generator.

Analytic Power has pursued fuel cell hydrogen generation via chemical hydrides for about five years. We have explored both hydrolysis and thermolysis methods. We have abandoned this line of R&D. Table 1 shows the specific weight and cost of several hydrogen sources along with the specific properties of the BA5590 battery. Analytic Power has recently demonstrated a prototype ammonia fuel processor. From the standpoint of simplicity and cost, ammonia is potentially the best hydrogen source for fuel cell power plants we have been able to identify.

Table 1 - Weight & Cost of Fuels

SOURCE	WHR/LB	cent/kWH	WHR/in3
H_2 GAS	7565	2353	4.62
NaBH4/NH_4Cl	668	1873	23.79
Mg +2 H_2O	282	17714	17.33
CaH_2 +H_2O	391	15596	26.82
METHANOL	660	379	18.87
DIESEL	469	34	14.63
NH_3	1077	93	2997
Propane	889	34	18.78
Butane	876	319	18.31
BA5590	70	34483	3.33

Table 1 shows the relatively high cost and low energy density of chemical hydrides. This is only one part of the problem. The second problem is the ratio of inactive to active (or fuel) weight and cost. While a chemical hydride fuel such as sodium borohydride starts out with a weight energy of 8.5% hydrogen, the weight of the control system and hardware reduce the fuel capacity to about 3%. This is no better than bottled hydrogen. Ammonia starts out with a hydrogen density of 17.5% and costs only a dollar a pound (retail). Because of its simpler reactor and storage system, the ratio of inactive to active weight with ammonia decreases as the energy storage increases. In the chemical hydride system, the ratio stays constant. Fuel cells make sense for missions where the amount of energy stored is large relative to the power required. In this situation, the weight of the fuel cell power system approaches the weight of the fuel (and tank). This condition is possible for ammonia or hydrocarbon fueled systems. It is not possible for chemical hydride systems.

The final problem with solid fuel reactors for small power plants is safety. The only way to guarantee safety is to limit the amount of fuel in the hydrogen generating reactor. This means separating the fuel storage from the reactor and the product storage. In the case of solid fuels, this generally results in cumbersome, expensive systems.

Most of the chemical hydrides are vigorously exothermic and can easily be used in thermoloysis. The problem is, most often, to reduce the heat release. While this can be done by adding excess hydride, the decomposition of the excess complex boron or aluminum hydride yields an alkaline hydride product (i.e. LiH or NaH). These hydrides are unstable and hazardous to handle. In the balance of this report, we will document our conclusions.

1.1 Objectives

The technical objectives of this program to develop a chemical hydride source for fuel cell hydrogen were focused at the areas of safety, heat release, parasite power consumption, and minimizing non-fuel weight. Specifically, a digital reactor development program must:

- Characterize the heat release of chemical hydrides from a digital reactor as a function of pellet composition and the use of accelerators and thermal sinks.
- Pellet ignition is crucial to the success of the digital reactor. Pellet initiation should be optimized from a cost and reliability standpoint.
- Minimize power consumption and non-fuel weight in the system
- Define a thermal management system that emphasizes safe operation of the hydrogen generation system.
- Define the control logic to implement the generator.
- Demonstrate how a 2.5 kWH system can be made with a weight of 5 lb. and a cost of $1000. Of this cost about half should be a non-recurring cost.

In addition to the digital reactor, we also explored these objectives for a hydride gun concept and a tape concept.

2. CONCLUSIONS AND RECOMMENDATIONS

2.1 Chemical Hydride Thermolysis Systems

The Digital Reactor concept using Beckert/Dengel chemistry is a solid reactant system. The problem with any solid reactant system is finding a method of moving the solid reactant from the storage section to the reactor section. This problem has been faced by the firearms manufacturers. We evaluated these approaches and found them to be too heavy and bulky. The alternative of using the reactant storage portion of the system as reactor and product storage system is unsafe. These conclusions can be extended to chemical hydrides in general. The final difficulty associated with chemical hydride systems is that they are all costly.

2.1.1 System Safety

The only safe way to provide hydrogen for a fuel cell is to limit the amount of hydrogen in the reactor at any time. In prior work, Analytic Power demonstrated successfully insulating reacting pellets from one another. As long as the triggering system worked properly, the system would be workable. Unfortunately, the triggering circuits of the system require solid state switches that can fail "closed." In this case it is not possible to guarantee that the pellet firing circuit was safe. While the Beckert and Dengel chemistry produces reaction products which are inert (unlike hydrolysis systems), it is possible to trigger more than one pellet at a time in the event of circuit component failure. This breeches the safety of the digital reactor.

2.1.2 System Weight

The objective of the project was to demonstrate a hydrogen generator that can supply 2.5 kWH, is easily portable weighs only 5 pounds, and is small enough to fit easily within a backpack. The weight of the fuel alone is 4 lb., leaving only 1 lb. for the igniters, insulation, electronics, and the container. If many small pellets are used, the packing efficiency of the fuel storage area is low, causing the hydrogen generator to be large. Each pellet needs an igniter. We intended to circumvent these problems by using quantities of gas yielding high pressures in a given storage volume, and smaller number of large pellets, measuring 1 inch in diameter, and 4 inches in length. However, large pellets generate high reactor pressure and thick containment vessels. Thick walled reactors increase the weight dramatically. We believe that it is impossible for a chemical hydride hydrogen generator to supply 2.5 kWH of hydrogen while weighing only 5 pounds.

2.1.3 Firearms Technology

A wealth of firearms technology is directly applicable to solids handling in chemical hydride systems. During this program Analytic Power worked with a gun smith to determine what solutions were available. Unfortunately, the weight of the cartridge shells and the gun are prohibitive in a power generating application. The noise and the problem of solid waste disposal do not auger well for this technology transfer either.

2.2 Recommendations

That work in the area of solid chemical hydrides should be terminated unless a low cost, high energy density, safe fuel is discovered. We have worked on the development of chemical hydride hydrogen generators for over five years. We have not found such a fuel and we believe that the chances of finding one are unlikely.

That work on fuels processing for small (50 to 500 watt) fuel cell power plants be focused on ammonia cracking, hydrocarbons processing and methanol.

3. SIMULATION AND ANALYSIS

3.1 Reaction Chemistry Solid Hydrides

The hydrogen generators are based on the substitution reaction of an ammonium compound with a complex hydride formed from an alkaline, or alkaline earth metals and either aluminum or boron. The anion of the ammonium compounds can be a halogen or a sulfate. In our case we used the chloride. The reaction chemistry has been described in a number of patents granted in the 1970's and 1980's to Werner Beckert and Ottmar Dengel among others. The patents were assigned to the US Navy. We will refer to the chemistry described below as "Beckert/Dengel" or "B/D" chemistry.
The Beckert/Dengel reaction uses the form:

$$m/n\ (NH_4)_nX + Y(ZH_4)_m \text{ --> } YX_{m/n}\ N + 4mH_2$$

where:
X is an inorganic acid group like a halogen or sulfate
Y is an alkaline or alkaline earth metal
Z is a trivalent metal capable of forming complex hydrides such as Al or B.
m is the valence of Z and n is the valence of X

For example, let X be chlorine, Y be sodium and Z be boron.

$$(NH_4)Cl + NaBH_4 \rightarrow BN + 4H_2$$

The heat released by this reaction is about 36 kCal/gmol. The heat release is unaffected by the reaction temperature. The change in Gibbs free energy increases as the temperature increases from about 66.5 kCal/gmol at 25 C to about 80.1 kCal/gmol at 427 C. This is because sodium borohydride decomposes at about 420 C.

Various additives can be mixed with the ammonium compound and the hydride to control the reaction rate and to control the heat release. Heat release is controlled by mixing alkaline or alkaline earth metal hydrides with the boron or aluminum complex hydrides. These materials decompose endothermically...We used this effect to limit the heat release of hydrogen pellets. In the experimental portion of the program we used excesses of lithium aluminum hydride ranging from 140 to 300%. While this limits the heat release, it renders the solid product reactive with water as lithium hydride is formed when the pellet is reacted.

The reaction rates used by Beckert & Dengel tend to be high, 100 liters being released by 100 gm of reactants in about 15 sec. Most of the reactants will attain roughly 1 liter of hydrogen per gram of reactants. The heat release tends to be high as well, about 500 joules/liter of hydrogen, although this can be significantly reduced.

The advantage of the B/D chemistry over other hydrides is that there is one solid phase reactant and one solid phase product. The only gas formed is the product hydrogen. Many

alternative hydrogen generator chemistries yield higher amounts of hydrogen per gram of reactants.

3.2 MicroFlo System Simulation

Simulations were performed on The fuel cell power plant unit and the fuel box hydrogen generator (see Figure 1). This analysis used Analytic Power's MicroFlo Code, which is a modular sequential systems analysis code for simulation. Sample printouts are attached at the end of the report for the power plant data, the chemical hydride performance, and the node array used by MicroFlo for a 150W plant.

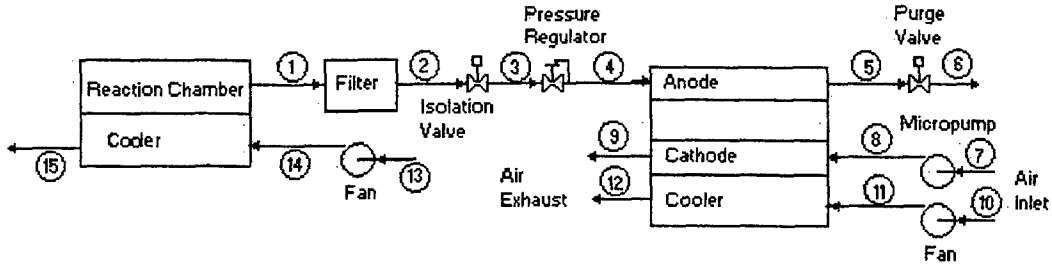

Figure 1: Fuel Cell Power Supply with Digital Reactor Hydrogen Supply

3.2.1 Fuel Cell

A simulation program was developed to calculate the flows of reactant streams flowing into and waste streams flowing out of the anode and cathode (labeled as streams 4, 5, 8, and 9 in Figure 1), depending upon the output power of the fuel cell. A heat balance was developed to calculate the flow rate of air necessary for adequate cooling of the fuel cell (the air coolant is represented as streams 10-12 in Figure 1).

3.2.2 Fuel Box

The simulation was expanded to calculate the heat released by the Beckert/Dengel (B/D) reaction using sodium or aluminum borohydride and ammonium chloride as reactants, as shown in Equation (1) and in Equation (2).

$$NH_4Cl + NaBH_4 \rightarrow BN + 4\ H_2 + NaCl \qquad (1)$$

$$NH_4Cl + LiAlH_4 \rightarrow AlN + 4\ H_2 + LiCl \qquad (2)$$

From this heat release, another energy balance was developed to calculate the flow of air to keep the Fuel Box at a constant temperature. This air could be supplied by the same fan that provides air to cool the fuel cell.

Because of the large amount of heat generated by the reaction in the fuel box, it is imperative to keep the heat away from unreacted material. The digital reactor concept involves keeping the heat generated by a reacted pellet away from the array of unreacted pellets that are mounted on a ceramic isolator on a circuit board. The insulation is the heaviest component in the digital reactor. Cooling a hydride gun is much easier. Since the heat is not evolved in the reactant storage space, it is safer than the digital reactor concept.

3.3 Calculations from THERMO Spreadsheets

A spreadsheet was developed to predict the temperature and pressure rise from the pellet reaction. The reason for the analysis is to predict the pressure and temperature which result from the thermolysis of a pellet. This information is requried to design a reactor to contain the pressurized hydrogen gas. The spreadsheets are shown in Tables 2 and 3The approach assumes that the generation of hydrogen gas with the simultaneous release of heat affects the reactor in two ways. Some of the energy is used to adibatically compress the gas to make space for the newly generated hydrogen. The energy that is not used in the compression process is dissipated by warming up the gases and the pellet. The energy release from the chemical reaction assumes that there is minimal decomposition of NH_4Cl. All of the NH_4Cl reacts with $LiAlH_4$, and excess $LiAlH_4$ decomposes endothermically to aluminum and lithium hydride. It is assumed that the temperature of the pellet and the gas generated are approximately equal. Over the course of the reaction, the quantity and composition of gas changes, and the composition of the pellet changes as the reaction proceeds.

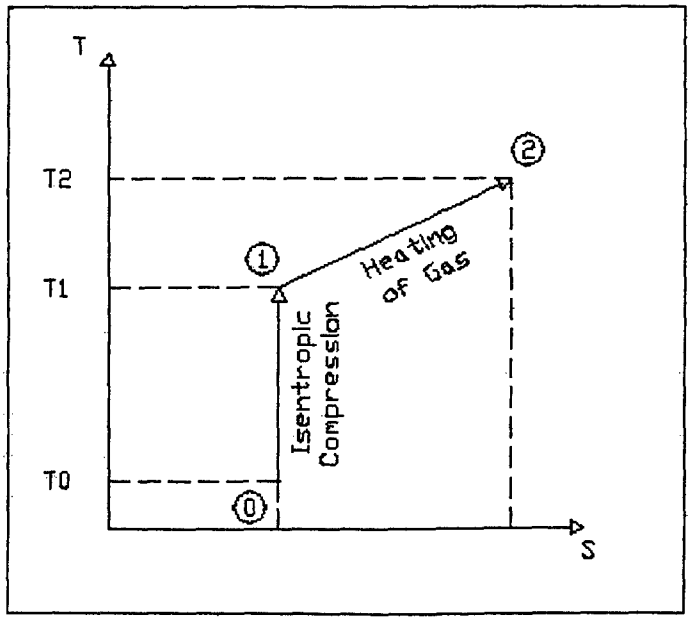

Figure 2: Thermodynamic Effects of Pellet Ignition

In Table 2, each row corresponds to an increment in the reaction progress variable (T. deDonder, see Physical Chemistry. G. Castellan, pg 137 or Principles of Chemical Equilibrium, K. Denbigh, pg 135) or extent of reaction. We have analyzed the process of pellet thermolysis as a series of processes that are illustrated in Figure 2. The first step is an adiabatic compression from state (0) to state (1). This is followed by a constant pressure heating from state (1) to state (2). Figure 2 schematically shows the process on a temperature entropy plane. In the spreadsheet shown in Table 3 we have broken the process into ten steps corresponding to an extent of reaction numbered 1 through 10. In each row we reach the state (2) from state (0). The spreadsheet analysis attempts to simulate a series of microscopically reversible states with a finite set of states. The series of states is nearly linear in the range of interest. For each row we evaluate intermediate

thermodynamic properties of the system as a small amount of fuel is consumed, releasing a small hydrogen gas element with a mass of δm and a heat energy increment ?h to the reactor volume. The correlation of the data with this model has not been good. Two reasons for the departure of the experimental data from the model are ammonium chloride decomposition and heating of the heavy steel experimental reactor shell.

Before reacting the pellet, the reactor was pressure tested with nitrogen and purged down to atmospheric pressure. The thermophysical properties of the gas must be of a mixture of H_2 and N_2. Fortunately, $c_p(H_2)$ = 20.53 J/mol-C ~ $c_p(N_2)$ = 20.69 J/mol-C. There is less than a 1% difference between these two values, thus the c_p values may be taken as constant. However the molecular weights are different ($MW(H_2)$ = 2.016 g/mol, and $MW(N_2)$ = 28.01 g/mol). The values for the average molecular weight and for the gas constant are calculated for each extent of reaction (row) as additional hydrogen is generated.

The heat capacity of the pellet is calculated from the value for the kraton rubber (since the rubber does not react, its' heat capacity is constant), the heat capacity for the initial quantity of reactants, and the heat capacity for the solid reaction products. Then the heat capacity for the pellet at any point in the reaction is calculated by

$$(mc_p)_{pellet} = (mc_p)_{kraton} + (1\text{-}x)(mc_p)_{reactants} + (x)(mc_p)_{solid\ products}$$

where x = fraction of reaction occurred
= (extent of reaction) / (total number of rows)

The pressure ratio $r_p = P_1/P_0$ may be calculated by the following equation:

$$r_p = \left(1+\frac{\delta m}{m}\right)^k$$, thus $P_1 = (r_p)*P_0$

Similarly, T1 is calculated with the following: $T_1 = T_0 * (r_p)^{\frac{k-1}{k}}$

The quantity of energy generated for each row $\Delta H_{0\text{-}2}$ is taken to be constant.
Because $\Delta H_{1\text{-}2} = \Delta H_{0\text{-}2} - \Delta H_{0\text{-}1}$, the value of $\Delta H_{0\text{-}1}$ may be used to find $\Delta H_{1\text{-}2}$.
Using thermodynamic values calculated already, $\Delta H_{0-1} = m_0 * c_p * T_0 * (r_p^{\frac{k-1}{k}} - 1)$.

Conservation of energy allows for the calculation of T_2 , and P_2 follows from the ideal gas law.

This spreadsheet has also been modified to predict the temperature and pressure rise within any closed vessel initially containing pure hydrogen by replacing the mixture molecular weight calculation with the molecular weight of hydrogen. This is useful for sizing an apparatus to react solid pellets of this Beckert/Dengel fuel.

The calculations developed by the spreadsheet suggest that the temperature rise of a pellet containing an excess of $LiAlH_4$ ought to have a lower temperature rise, but experimental data has not agreed with this. This is probably due to NH_4Cl decomposition. Although the number of moles of NH_4Cl that decomposes is small for either the 40% or the 200% excess mixture of $LiAlH_4$, it is more endothermic than the $LiAlH_4$ decomposition. The temperature rise observed experimentally is due to the balancing of reduced NH_4Cl decomposition with increased $LiAlH_4$ decomposition for the mix with the greater amount of $LiAlH_4$. The results of the analysis were used to generate the pressure and temperature graphs shown in Figures 3 and 4. These figures show the final pressure and temperature which is expected from the complete reaction of a pellet with a given starting mass and excess fuel. Comparing the two figures we note that the addition of 200%excess fuel drops the final temperature and pressure significantly when compared to a 25% excess.

Table 2
System Thermodynamics
(reservoir previously contained N_2):

Gun Reservoir Thermodynamics: for a mixture of N2 and H2 gas									
Solution of Pellet Reaction									
Vo	1	liter =	61.0234	in3	k	1.405		k/(k-1)	3.469136	
pellet m	2.5	gm	0.005511	lb	cp	3.421	btu/lb-F	(k-1)/k	0.288256	
alpha	2				cv	2.4354	btu/lb-F	n_NH4Cl	1.269E-02	g_moles
m_initial	1.1456	gm	2.526E-03	lb	To	530	R	(mcp)fuel	2.312E-03	btu/deg.R
n	10				delm*hf	0.332542		(mcp)sp.f.	1.221E-03	btu/deg.R
delm x n	0.205906	gm	4.539E-04	lb	del hf	-7325.71	btu/lb h2	(mcp)krtn	2.729E-04	btu/deg.R
delm	2.06E-02		4.539E-05		Po	1	atm			
plt. Kr.	15%		1.797%							

Extent of Rxn.	mo+delm lb_m	av. MW lbm/lbmol	R0(mxtr.) btu/lb-F	R1(mxtr.) btu/lb-F	Vo(cv/R+1) btu/atm	1+delm/mo	mcp_plt btu/deg.R	rp	p1 atm
1	2.571E-03	22.8158	0.071787	0.087089	2.783225	1.01797	0.00248	1.025345	1.025
2	2.616E-03	19.35172	0.087089	0.102678	2.375243	1.01766	0.00237	1.024896	1.190
3	2.662E-03	16.87676	0.102678	0.117736	2.083753	1.01735	0.00226	1.024462	1.370
4	2.707E-03	15.02019	0.117736	0.132289	1.865096	1.01705	0.00215	1.024043	1.563
5	2.753E-03	13.57599	0.132289	0.146361	1.695005	1.01677	0.00204	1.023639	1.771
6	2.798E-03	12.4205	0.146361	0.159977	1.558917	1.01649	0.00193	1.023248	1.994
7	2.843E-03	11.47502	0.159977	0.173159	1.447563	1.01622	0.00182	1.022869	2.234
8	2.889E-03	10.68706	0.173159	0.185926	1.354761	1.01597	0.00171	1.022503	2.490
9	2.934E-03	10.02028	0.185926	0.198298	1.276231	1.01571	0.00160	1.022148	2.763
10	2.980E-03	9.448729	0.198298	0.210293	1.208916	1.01547	0.00149	1.021805	3.052

Extent of Rxn.	To R	T1 R	h in btu	h 0-1 btu	h 1-2 (tot) btu	p2 atm	T2 R	H1-2gas btu	H1-2plt btu
1	530	440.0402	0.332542	0.033157	0.299385	1.161105	498.3037	0.512443	-0.07847
2	498.3037	425.6538	0.332542	0.031177	0.301365	1.336919	478.2008	0.470326	-0.04757
3	478.2008	419.9574	0.332542	0.029922	0.30262	1.526003	467.9072	0.436625	-0.02324
4	467.9072	419.2958	0.332542	0.02928	0.303262	1.729677	464.1003	0.414941	-0.00818
5	464.1003	422.3114	0.332542	0.029045	0.303498	1.94876	464.8141	0.400225	0.001456
6	464.8141	428.0791	0.332542	0.029092	0.303451	2.183776	468.8058	0.389825	0.007706
7	468.8058	435.9513	0.332542	0.029344	0.303199	2.435067	475.2481	0.382242	0.011734
8	475.2481	445.4624	0.332542	0.029749	0.302793	2.70285	483.568	0.376572	0.014247
9	483.568	456.2698	0.332542	0.030272	0.30227	2.987265	493.355	0.372247	0.015892
10	493.355	468.1158	0.332542	0.030887	0.301655	3.288389	504.3069	0.368893	0.016365

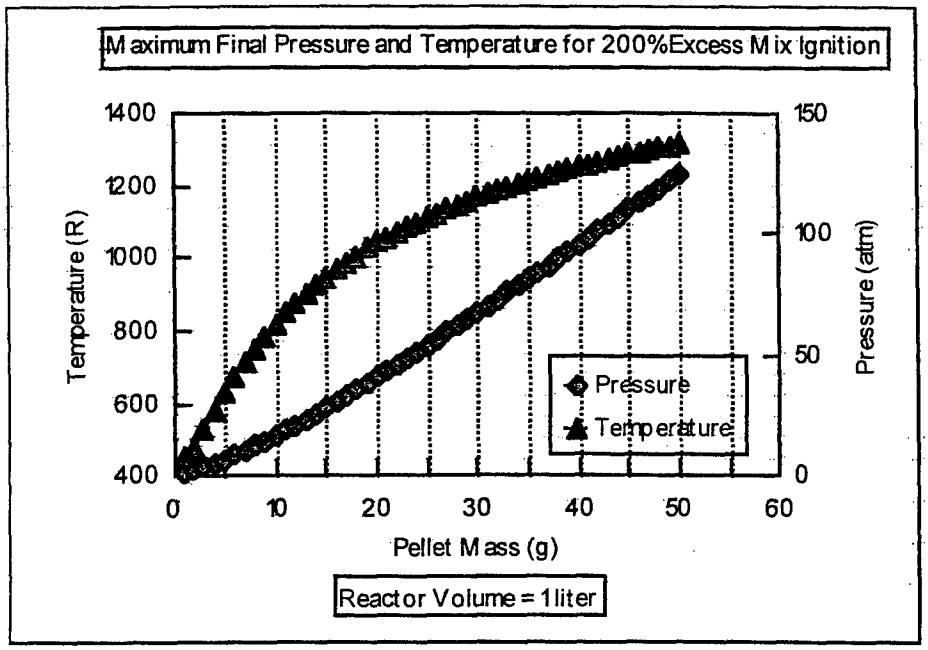

Figure 3

Table 3
System Thermodynamics

Gun Reservoir Thermodynamics: for pure H2 gas
Solution of Pellet Reaction

Vo	1	liter =	61.0234	in3	k	1.405		k/(k-1)	3.469136	
pellet m	44	gm	0.097002	lb	cp	3.421	btu/lb-F	(k-1)/k	0.288256	
alpha	0.39				cv	2.4354	btu/lb-F	n_NH4Cl	3.471E-01	g_moles
m_initial	0.083443	gm	1.840E-04	lb	To	530	R	(mcp)fuel	3.778E-02	btu/deg.R
n	10				delm *hf	10.73589		(mcp)sp.f.	1.802E-02	btu/deg.R
delm x n	3.689278	gm	8.133E-03	lb	del hf	-13199.9	btu/lb h2	(mcp)krtn	4.804E-03	btu/deg.R
delm	3.69E-01		8.133E-04		Po	1	atm			
plt. Kr.	15%		442.123%							

Extent of Rxn.	mo+delm lb_m	MW H2 lbm/lbmol	R0(mxtr.) btu/lb-F	R1(mxtr.) btu/lb-F	Vo(cv/R+1) btu/atm	1+delm/mo	mcp_plt btu/deg.R	rp	p1 atm
1	9.973E-04	2.016	0.985615	0.985615	0.333525	5.42123	0.04061	10.74997	10.750
2	1.811E-03	2.016	0.985615	0.985615	0.333525	1.81554	0.03863	2.311549	19.077
3	2.624E-03	2.016	0.985615	0.985615	0.333525	1.44920	0.03666	1.684167	33.153
4	3.437E-03	2.016	0.985615	0.985615	0.333525	1.30996	0.03468	1.461334	51.353
5	4.251E-03	2.016	0.985615	0.985615	0.333525	1.23662	0.03271	1.347696	73.452
6	5.064E-03	2.016	0.985615	0.985615	0.333525	1.19134	0.03073	1.278888	99.321
7	5.877E-03	2.016	0.985615	0.985615	0.333525	1.16061	0.02875	1.232779	128.849
8	6.691E-03	2.016	0.985615	0.985615	0.333525	1.13839	0.02678	1.199739	161.943
9	7.504E-03	2.016	0.985615	0.985615	0.333525	1.12156	0.02480	1.174904	198.510
10	8.317E-03	2.016	0.985615	0.985615	0.333525	1.10839	0.02283	1.155558	238.467

Extent of Rxn.	To R	T1 R	h in btu	h 0-1 btu	h 1-2 (tot) btu	p2 atm	T2 R	H1-2gas btu	H1-2plt btu
1	530	1050.958	10.73589	0.327855	10.40803	8.252702	806.8158	-0.83295	11.24093
2	806.8158	1027.24	10.73589	0.752029	9.983858	19.68486	1059.997	0.202905	9.780965
3	1059.997	1231.861	10.73589	1.06455	9.671338	35.14094	1305.743	0.663205	9.008172
4	1305.743	1456.625	10.73589	1.354401	9.381486	54.50222	1545.963	1.050527	8.331021
5	1545.963	1684.825	10.73589	1.632876	9.103012	77.66165	1781.374	1.40396	7.699134
6	1781.374	1912.275	10.73589	1.903474	8.832414	104.5195	2012.373	1.734085	7.098431
7	2012.373	2137.503	10.73589	2.167729	8.568159	134.9816	2239.23	2.045339	6.52294
8	2239.23	2359.912	10.73589	2.42647	8.309418	168.9586	2462.153	2.340152	5.969404
9	2462.153	2579.251	10.73589	2.680216	8.055671	206.3655	2681.316	2.620118	5.435707
10	2681.316	2795.427	10.73589	2.929332	7.806555	247.1209	2896.87	2.886418	4.920308

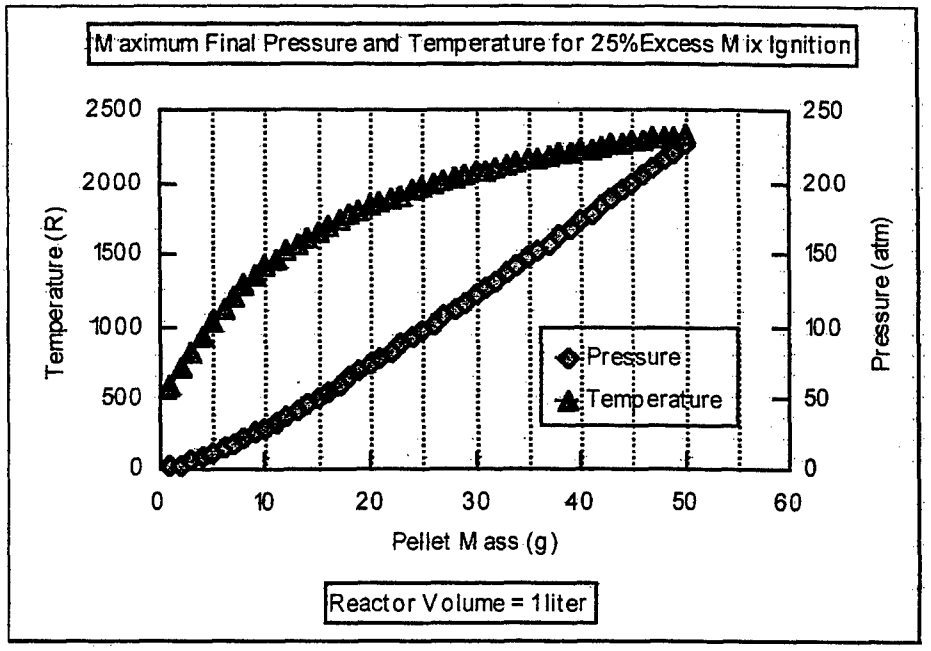

Figure 4 Sample Results for System Thermodynamics (reservoir previously contained H_2)

4. EXPERIMENTAL

4.1 Results

In the course of this program, ten chemical hydride pellets ranging in weight from about 2.5 gm to 14.5 gm were prepared and fired. The pellets, which were $LiAlH_4$ and NH_4Cl, varied in composition from about 1.4 stoichiometric (40% excess $LiAlH_4$) to 300% stoichiometric. The objective of the additional hydride is to absorb the heat of reaction with the endothermic heat of $LiAlH_4$ decomposition. The reactions involved are shown in Table 4.

Table 4 Hydrogen Generation Reactions

Equation No.	Reaction	$?H_{rxn}$(298K), kcal/g mol
1	$NH_4Cl + LiAlH_4 \rightarrow 4\ H_2 + LiCl + AlN$	- 69.60
2	$LiAlH_4 \rightarrow Al + 1.5\ H_2 + LiH$	+ 6.34
3	$NH_4Cl \rightarrow NH_3 + HCl$	+ 42.95

The results using pellets of varying fuel compositions are shown in Table 5. These pellets have $LiAlH_4/NH_4Cl$ molar ratios of 1.4:1 and 3:1. Thermodynamic calculations based on the heats of formation show that the reaction of $LiAlH_4$ and NH_4Cl (Reaction 1 in Table 4) is exothermic. Decomposition of the excess $LiAlH_4$ (Reaction 2 in Table 4) is endothermic and it absorbs much of the heat generated by the competing reaction of $LiAlH_4$ and NH_4Cl. Generation of NH_3 by the decomposition of NH_4Cl (Reaction 3 in Table 4) is reduced with an excess of the $LiAlH_4$ because this reaction does not include $LiAlH_4$ as a reactant. The NH_4Cl decomposition reaction occurs at a higher temperature

than the $LiAlH_4$ / NH_4Cl reaction. The $LiAlH_4$ decomposition reaction is endothermic. The NH_4Cl decomposition is discouraged by other endothermic reactions. Since the decomposition of $LiAlH_4$ is also endothermic, an excess of $LiAlH_4$ will minimize ammonia generation. Unfortunately, the excess of LiAlH4 yields LiH in the product solid. This compound is sensitive to water. This will result in product disposal problems.

During our experiments, several pellets misfired. This was generally due to a broken bridgewire or low pellet density. The recommended value for the pellet density is 20 g/in^3.

An important characteristic is the time interval between pellet firing and the start of the reactor pressure rise. This time interval was found to vary between 7 seconds and 1.8 minutes. The firing time interval must be minimized for two reasons: one, the ammonium chloride decomposes at elevated temperatures creating undesirable gases and reduces the H_2 yield; and two, more electrical energy is needed to initiate each reaction. This places a greater electrical power drain on the output of the fuel cell and requires more electrical energy for start up.

Table 5: Ignition Results

Reactant Mixture	Mass (g)	Pressure Rise (psi)	Temperature Rise (F)	Pressure Rise (psi)
1.4:1	2.55	29	34	11
1.4:1	2.7	27	30	10
3:1	2.2	31	38	14
3:1	2.5	36	34	14
3:1	2.52	32	30	13
3:1	2.6	35	50	13
3:1	5.2	63	36.6	12
3:1	5.35	66	18.5	12
3:1	5.7	72	44.1	13
3:1	7.4	105	285	14
3:1	14.3	180	16.1	13

4.2 Pellet Ignition Procedures

Pellets were ignited in a one-liter reactor. The reactor is a four inch diameter stainless steel pipe about 6 inches long. It has threaded pipe caps on either end. The reactor is leak tested prior to ignition. The pressure rise for a pellet 2.5 - 2.7 g is about 30 psi and the maximum gas temperature measured is 100 F. This gas is rapidly cooled by expansion and heat transfer to the reactor wall. A small temperature increase is observed in the reactor wall (the temperature rise is too small to measure for a 2.5 g pellet). For larger pellets, the steel has occasionally risen about 7 F. The reactor has been successfully pressure tested up to 1000 psi with nitrogen gas. The reactor is equipped with gages with a "tell tale" to measure the maximum pressure reached during the reaction. The reactor also has a feed-through with J-type thermocouples and ignition current wires. The current needed for ignition depends on the thickness of the wire. For example, 28 gauge (13 mil) Ni-Cr wire needs about 3-4 A.

We recorded the following data on each run:

- pressure and temperature (both prior to and after the ignition)
- time interval between firing and reactor pressure rise
- time B/D reaction termination
- ignition voltage and current

When all of the measurements have been taken, the reactor is opened into a fume hood. After the reactor reaches atmospheric pressure, it is re-pressurized with nitrogen and bled again into the fume hood to remove the remaining vapors before it is opened. After the fumes have dissipated, the endcap is loosened and removed. The spent fuel usually appears much darker than the original pellet, and is twisted or stretched.

5. FUEL PROCESSOR DESIGNS

In this section we will describe the approaches pursued in the development of the thermolysis of chemical hydrides. All of the thermolysis reactors used the reaction chemistry defined by Beckert and Dengel.

5.1 Digital Reactor

5.1.1 Configuration and Ignition

The Digital Reactor is built from chemical hydride pellets. The pellets are placed in an array on a board (see Figure 5 below). Each pellet contains a bridgewire for ignition.

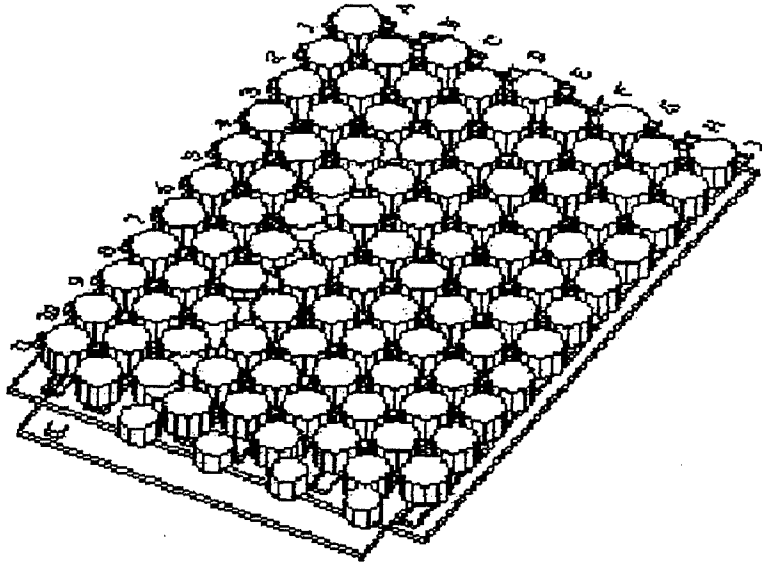

Figure 5: Digital Reactor

The bridgewire of each pellet is connected to a wire array shown in Figure 5. An electronic control can address each pellet to be fired by placing a firing voltage on a row and a ground on a column of the array. The approach has much in common with core memories which were once used in computer memories. The result of addressing the pellet

in this manner is that current flows through only the pellet bridgewire in the energized row and the grounded column. The current must heat the wire to the ignition temperature for the B/D reaction. Typically the pellets were ignited by passing current through a 8 mil Nickel-chromium bridgewire installed along the cylinder axis of the pellet. The resistance prior to ignition was measured to be 3.5 Ω.. The current was gradually increased and the current that successfully ignited the pellet was 1.7 A, corresponding to a voltage of 6.0 V. Various thermo-chemical amplifiers were investigated such as thermite, and perchlorates. None was adjudged safe.

The interpellet space must be insulated and a cooling system is needed to prevent the heat released by a reacting pellet from igniting adjacent pellets. Failure of the insulation would result in a chain reaction that would fire all the pellets, causing the fuel box to explode. To be safe, a reactor design would require a method of preventing such an event. The problem is complicated by the fact that the transistors, which could be used in the firing circuits, often fail closed. This would cause firing of several circuits. This is the principal reason for abandoning the fuel box approach to a digital reactor.

5.1.2 Fuel Box Packaging

Assuming a pellet size of about 0.625 in. diameter and 0.5 in. high, we can fit about 162 pellets on a 13.375 x 5.75 inch board. Four such boards can fit in an aluminum box. The energy capacity of a box about this size is 2.5 kWH. Boxes can be made larger or smaller to provide different energies. The pellet interstices are filled with a porous calcite furnace insulation that insulates the firing pellet from its neighbors. The inter-pellet volume serves as a hydrogen reservoir. The reservoir volume is generally designed to limit the pressure rise caused by igniting a pellet to a pressure less than 60 psi. This pressure is set by the pellet size and igniter weight and cost. The larger the pellet, the more hydrogen will be released per firing. With small pellets, the igniter will constitute an increasing fraction of the system weight and cost.

Table 1 shows the weight and cost breakdown of a 2.5 kW digital reactor fuel box. The weight and cost are broken into the pellet ingredients and internal fixtures. These are assumed to be non-recoverable when the pellets are discharged. The external fixtures are permanently mounted on the fuel cell power plant. The expense of the external fixtures is a non-recurring expense. The hydrogen produced by this unit is projected to be about 135 gm. Since the weight of the complete box is about 8.1 lb., the hydrogen density is only about 3.65%. One of the primary research objectives was to improve the hydrogen density. Since many of the elements of the fuel box do not scale with energy, the higher the energy required of a fuel box, the higher the hydrogen density. As the energy required of the system increases, the weight of the system approaches the weight of the fuel and insulation. In the case of the reactants we use, this can be about 8.6%.

At first glance, it might appear that the hydrogen density is quite low. This is because investigators do not include the complete inactive weight in their calculations. For example, we have delivered a gaseous hydrogen system to the Dismounted Battlespace Battle Lab. These systems are often quoted as being about 5.6% by weight hydrogen at

6000 psi. Since our system was a 3000 psi system we would expect a number like 2.82%. In fact we attained 1.68%. But this system included burst disks, a regulator, CGA fittings, etc. Reversible metal hydride systems are often quoted as having 1% by weight hydrogen storage for Fe/Ti hydrides. This is the weight of the alloy only.

5.1.3 Heat Release

The heat release of a 2.75 gm pellets is about 2.5 BTU or about 2575 joule. At a hydrogen evolution rate corresponding to a fuel cell power output of 150 watt, the digital reactor produces about 43 watts (150 btu/hr) of waste heat. To put this in perspective, the fuel cell stack operating at 150 watts produces about 118 watts (400 btu/hr) of heat. While this is not a big heat load, we must be prepared to deal with it because the accumulation of heat in the digital reactor could cause premature firing of the pellets or decomposition of the ammonium chloride. The latter could damage the fuel cell stack.

The cost of the fuel is about 23$/kWH vs Li batteries such as the Army BA5590 which is 287 $/kWH (not counting disposal cost). Most studies of chemical hydride fuels use the cost of sodium borohydride but actually use lithium borohydride in their experiments. Lithium borohydride which is made from sodium borohydride, is an order of magnitude more expensive than sodium borohydride.

5.2 Hydride Gun

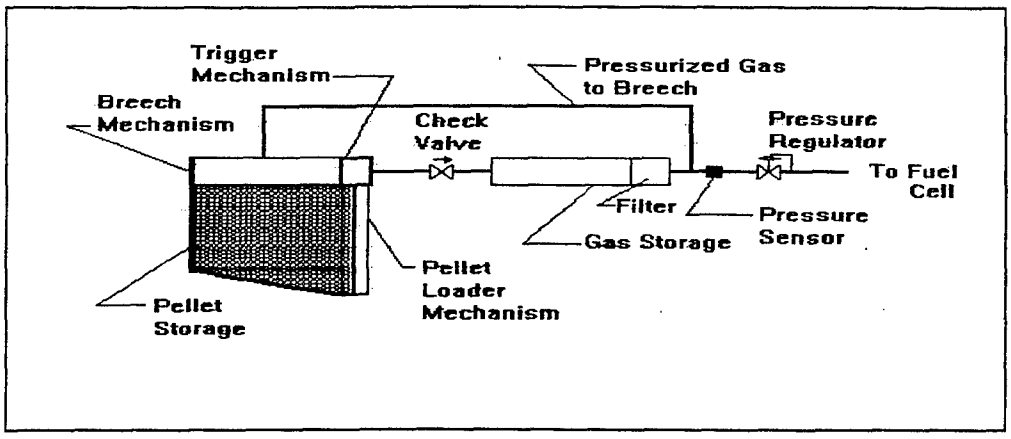

Figure 6 *Schematic of the Hydride Gun*

The hydride gun concept was developed as an alternative to the digital reactor. The hydride gun concept was studied because it solves a fundamental safety problem of the digital reactor. In this concept, fairly large pellets (cartridges) are moved from a storage location (magazine) to a separate reactor (chamber) for firing. The solid product of the reaction is discharged from the chamber prior to loading the next pellet. The configuration is shown in Figure 6. Pellets are transported from the storage magazine to a breech where they are fired. The trigger mechanism is electronically actuated when the anode pressure is low. The pellet releases about five grams of hydrogen on firing. This is stored in a high pressure bottle. The thermolysis reaction is capable of generating high pressures. The

Table 6 Weight and Cost Breakdown of Digital Reactor

Part Description	quantity	total weight lb	total cost
pellet ingredients			
NaBH4	1	1.543	$31
NH4Cl	1	1.876	$24
Kraton thermoplastic rubbe	1	0.000	$7
mineral oil	1	0.171	$7
toluene	1	0.051	$8
pellet igniters	648	0.324	$162
Subtotal		3.966	$239
internal fixtures			
reactor housing	1	0.500	$20
circuit boards	4	0.400	$60
card guides	4	0.080	$4
insulation	4	1.525	$72
board connectors	4	0.040	$56
Subtotal		2.545	$211
external fixtures			
on/off switch	1	0.010	$15
Box	1	0.500	$5
on/off indicator (green)	1	0.001	$4
fuel low indicator (yellow)	1	0.001	$4
auto shutoff indicator (red)	1	0.001	$3
board relay	1	0.120	$4
power source	1	0.100	$12
pressure transducer	1	0.110	$30
pressure control switch	1	0.100	$75
pressure transducer	1	0.100	$30
pressure gauge	1	0.100	$12
pressure regulator	1	0.070	$0
pressure relief valve	1	0.080	$30
teflon tubing	1	0.050	$3
female quick disconnect va	2	0.100	$10
male quick disconnect valv	2	0.080	$10
external cable	1	0.010	$10
logic units	1	0.100	$420
Subtotal		1.633	$678
services			
insulation machining			
board fabrication			
pellet fabrication			
logic circuit			
totals		8.144	$1,128

only by the power of the fuel cell and the pellet size.

pressure of hydrogen in the gas storage cylinder is used to drive the breech loading and discharge mechanism.

5.2.1 Fuel Storage

The fuel is separate from the reaction chamber and is stored as cylindrical pellets 1 inch diameter and 4 inches long, yielding about 5 grams of hydrogen gas when initiated. Pellets are stored in a spring loaded magazine. Since the pellet storage is separate from the reactor the energy storage portion of the system can grow independently from the reactor. The reactor size is determined by the power of the fuel cell.

5.2.2 Pellet Loader

The pellets are dispensed from the bottom end of the pellet storage magazine. The pellets are carried to the breech via a spring such as found in machine guns. The pellet caliber and the power of the fuel cell power plant determine how rapidly the gun must fire.

5.2.3 Reactor

The reactor consists of the breech and firing chamber and the gas storage and filtration system. The reactor size is determined

5.2.4 Breech & Firing Chamber

The breech and firing chamber are similar to those found in guns. The pellet is driven into the chamber by the pellet immediately behind it. The breech mechanism is gas pressure driven from the hydrogen gas storage bottle. The firing chamber is subject to high pressure. The pressure is determined by the maximum pressure in the gas storage bottle. The firing chamber is fitted with a check valve so that the product hydrogen gas, which is stored at high pressure, does not leak out through the firing chamber when the breech is opened to admit the next pellet.

5.2.5 Ignition

Ignition can be electric or percussion. Pellet ignition is one of the more difficult parts of this project. Ignition is crucial to the process because the ammonium chloride will decompose into ammonia and hydrochloric acid if even a short time is spent at an elevated temperature.

5.2.6 Gas Storage and Filtration

The pellet fires into a gas storage cylinder. The volume of the gas storage cylinder is set by the volume of gas evolved by the pellets. The gases are evolved at very high pressures (several hundred psi) which means that the gas storage volume is low. Spent pellets are simply ejected into a product storage container after firing. If the pellets are cooled with excess hydride it may not be feasible to simply eject the pellets because the spent pellet, which contains an alkaline hydride, will further react with water. The gas product itself is fed to a charcoal or zeolite filter allowing only hydrogen into the fuel cell.

5.2.7 Check Valve

A check valve is interposed between the pellet and the gas storage bottle. The check valve will be subject to severe duty since the gas evolved will be at high pressures and elevated temperatures. We have estimates of the gas storage bottle temperature but not the breech. It may be advisable to place an additional filter upstream of the check valve to prevent particles from being carried into the valve where they could hold the seat open.

5.2.8 Product Storage & Disposition:

One approach is to have a flexible storage bag to catch spent pellets ejected from the breech. If we follow this approach, it might make the use of cartridge shells feasible as well. In this case we would simply be ejecting something very like a spent shell.

An alternative approach would be to return the spent reactants to the unreacted pellet storage chamber. This minimizes the system volume. If the pellets are hot when they are ejected, pre-ignition of unreacted pellets could occur..

5.2.9 Control

The control system is quite simple. A pressure transducer is mounted on the gas bottle, or immediately downstream from the gas bottle. When the pressure in the gas bottle drops to

some predetermined value, a logic circuit determines that a pellet is loaded into the firing chamber. If the pressure regulator delivers gas at about 5 psi to the anode, we will probably require a minimum pressure of about 20 psi in the gas storage bottle. When the pellet is in the chamber, the firing mechanism must be activated and the pellet discharged. Since the bottle contains the highest pressure immediately after pellet firing, it makes sense to insert a new pellet into the firing chamber at this time.

5.3 Tape Feeder

The separation of the reactant storage and the reactor components allows a cooling system to be developed to direct the reactor heat to the atmosphere, and away from the reactant storage. The key issue in solid fuel systems is the transportation of fuel to the reactor and transportation of products from the reactor. This must be accomplished with a minimum of parasitic power. The apparatus must also be kept small and lightweight for easy user mobility.

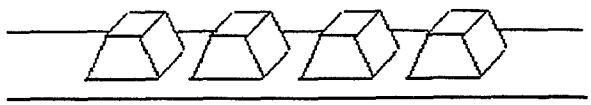

Figure 7: Tape for Feeding Fuel

Another design considered involved depositing the reactants in a slab on a tape (see *Figure 7*). This will allow for a pressure or electric driven motor to control movement of reactants into the reaction chamber and products out of the chamber. The spent reactants may then be removed one of three ways:

1) Moving them into a separate chamber for storage of waste products
2) Disposing of them outside of the apparatus
3) Bringing them back into the chamber where the reactants were originally stored (see Figure 8).

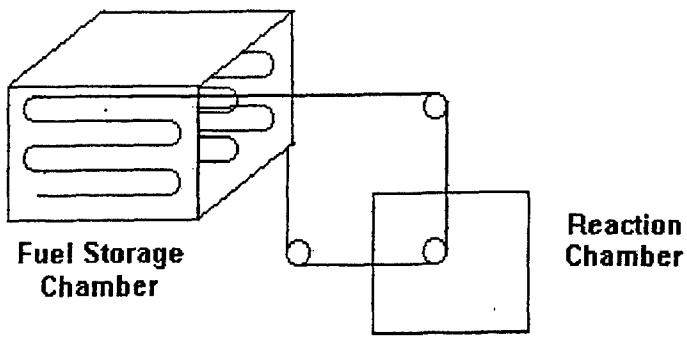

Figure 8: Tape feeder with return of spent fuel

The first option is undesirable because it would increase the size of the apparatus. The second option would have the undesired effect of littering the area where the system is used, as well as requiring an additional device to cut off the tape containing the spent reactants. Therefore, the design that returns the spent reactants appears to be the best way to make a tape feeder.

A variant of the tape feeder is the rolled tape feeder concept. It involves spinning the tape into rolls, similar to the manner in which the tape is stored within audio cassettes (see Figure 9). Calculations were made for the necessary volume for the rolls, assuming each individual pellet was shaped as a rectangular block (dimensions: 1.6 in x 0.31 in x 0.31 in), with the longest side in the axial direction of the roll. The spacing between each block is 0.31 inch, and the rod that the tape is wrapped around has a 4 inch diameter, the total diameter of the roll when at its fullest wrapping is 12.9 inches. When it is half unwrapped the diameter is 9.5 inches. This is small enough that it may be feasible for the chemical hydride H_2 generator.

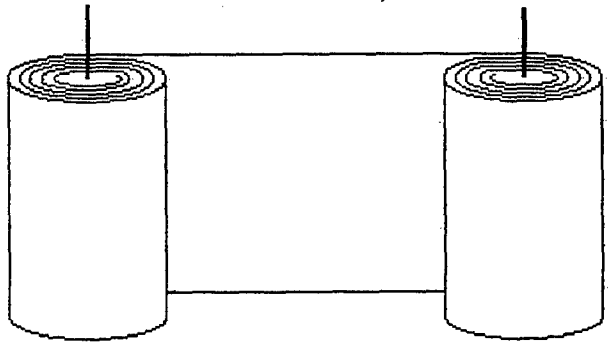

Figure 9: Rolled Tape

If each pellet were shaped as a cube with 0.53 inches on each side, the diameter of the roll for the case above would be 22 inches, which would undermine the compactness and mobility of the device.

A drawback, which is inherent in all the tape-feeding designs, is the necessity for a motor to spin a reel to wind the tape. The power to run a motor would be a parasitic load on the fuel cell. This tape-feed has the advantage of requiring only one motor, unlike other designs which have been considered. The autoloading hydride gun approach requires no motors to accomplish loading.

6. IGNITION METHODS

All pellets ignited during this project were ignited by passing electrical current through a bridgewire. The advantage of this approach for the final product is that this electrical power may be drawn from the electrical output of the fuel cell stack. Supplying electrical power during start-up requires a battery. The battery could be a primary, or a secondary recharged by the fuel cell. An alternative is to have the hydrogen tank/reservoir contain a supply of hydrogen gas when not in use. The tank contains enough hydrogen to permit the fuel cell to deliver to start and to provide ignition power to the hydride gun. For the hydride gun, pellets are moved around. The pellets have bridgewire ends projecting from the pellet body. The problem of connecting the bridgewire ends to an ignition source in the breech has not been addressed. This is not a trivial problem. It is made more difficult if the pellet is fabricated without some kind of shell.

6.1 Percussion Ignition

Percussion involves striking the fuel with an adequate force to initiate the reaction. This approach is common in conventional firearms and could be easily implemented in the hydride gun.. This approach demands the pellet and the ramming component be designed so that the hammer will strike with the all-fire energy, and the no-fire energy is be kept high enough to prevent premature ignition while the pellet is being loaded. Start up of a

hydrogen generator employing percussion ignition of hydride pellets would not require storage of electrical energy within a battery, but would require storage of mechanical energy to generate the initial ramming force to ignite the first pellet. Were this to be developed, the all-fire ramming force would have to be small enough that it could be initially created by a spring, or some other device to store mechanical force. The spring would need to be compressed prior to each start up of the hydrogen generator, so the procedure for interrupting the device operation would need to include compressing the spring, which could be done by the H_2 gas pressure. This percussion device could be modified by adding an outer shell to protect the reactive materials within the pellet from moisture and handling. The ramming force would then break the shell, and initiate the reaction. We expect that a shell would add considerably to the weight of the pellet. However, recently developed NATO ammunition is fabricated without a shell. An outer shell, on the other hand, protects the reactive materials from moisture and handling.

Bullets in conventional firearms employ lead azide primer. This primer reacts when struck by the hammer, generating enough energy to ignite the gunpowder. Use of a lead azide primer would be unacceptable for a hydrogen generator because the reaction it undergoes (Equation (3)) generates lead particles. If not removed, they will poison the fuel cell anode.

$$Pb(N_3)_2 \rightarrow Pb + 3\ N_2 \qquad (3)$$

With the heightened concern about the adverse effect of lead on people shooting within indoor firing ranges, ammunition manufacturers are developing primers that will generate products which are safer than those produced by lead azide. Most of these alternative primers are trade secrets kept by the ammunition manufacturers. For example, Remington has a product called Leadless™ ammunition, which their representative says is patent pending. Once the patent is issued they will be able to discuss what is in their product. The only manufacturer that we found who was willing to discuss their non-lead alternative primers was CCI in Lewiston, ID who has patented their primer. They use diazodinitrophenol as the initiator, tetracene as their secondary explosive, a mixture of nitrocellulose and nitroglycerin as the fuel, and strontium nitrate as their oxidizer. Tetracene (naphthacene) has a molecular formula of $C_{18}H_{12}$, with a structure (see *Figure 10*) of four adjacent benzene rings. The Merck Index did not specifically list diazodinitrophenol, but it clearly is aromatic. Most organics will poison fuel cell anodes so this material is problematic.

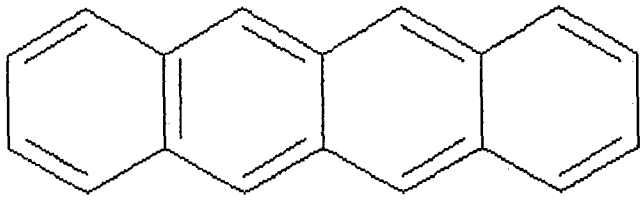

Figure 10: Structure of Tetracene

It may be possible to ignite the Beckert/Dengel fuel mixture directly by percussion, without the need of a primer. A new reactor could be built to subject a fuel sample to percussion and contain the reaction, while with adequate instrumentation to measure the results.

6.2 Percussion Piezoelectric Crystal

This involves a ramming device with a piezoelectric crystal inside that converts the ramming force into electricity. The electricity is sent through a bridgewire, which ignites the pellet. The problem with this approach is that it often takes quite a while to get a B/D reaction going. We expect that a thermochemical amplifier would be required as in the case of percussion igniters.

6.3 Surface Conduction

The ignition may be effected by conducting electricity through the surface material. The pellet will be coated with an conductive material that would generate enough heat to ignite an adjacent material. The inner core would be the Beckert/Dengel reactants. Iron might be an interesting material in this case. Work by Beckert and Dengel shows that metals tend to slow the thermolysis reaction. Metal oxides tend to speed the reaction but they are generally non-conductors.

6.4 Bridgewire Surface

The ignition is caused by a bridgewire that makes direct contact with the outer shell of the pellet. In this case the outer shell must be made of a material that is able to protect the inner fuel from moisture and mechanical stresses from the loading process, and it must be attain a temperature high enough to ignite the fuel mixture.

6.5 Bridgewire Penetration:

Ignition is caused by a bridgewire that punctures the protective outer coating of the pellet and makes direct contact with the layer of primer material, beneath the outer coating. The fuel is stored at the core of the pellet. The problem with this approach is that although a thin bridgewire is desired to reduce the energy pulse necessary to cause ignition, a thin bridgewire would probably be susceptible to being broken.

7. EXPERIMENTAL PROCEDURES

7.1 Preparation of Fuel Pellet Powder

The following is the procedure developed by Analytic Power for the safe preparation of fuel pellet powder. Deviation from the procedure is discouraged due to the reactive nature of the chemical hydrides.

7.1.1 Setting up the Glove Box

Select the correct recipe proportions based on desired hydride, percent excess hydride, and percent binder and plasticizer. Use the "recipe spreadsheet."

The glove box should contain the following in preparation for mixing:

Ingredients: $LiAlH_4$, NH_4Cl, Kraton (Binder)
Desiccant: Phosphorus pentoxide (P_2O_5)
Syringes, Scale [if possible], Weighing Pans, Scoopula
Dry Cloth, Paper Towels
Wooden stick, Disposable Spoons, or Glass Stirrer
Mixing Beaker, Trash Beaker
Watchglass (to contain desiccant)
Hamilton Beach Drink Master to mix fuel
Cans and hammer
Fill the dry box with nitrogen gas

7.1.2 Mixing the Solids

- Spread phosphorus pentoxide (P_2O_5) out on watchglass to dry the environment inside box.
- Weigh out necessary quantities of solid ingredients (use weighing dishes for the solids; add the liquids later under the fume hood).
- Safety comments: if any powder is spilled, pick it up with dry paper towels and store in a beaker.
- Mix solid ingredients with drink mixer. Have drink mixer on low and short pulses at all times (the powder must not be heated). First add NH_4Cl, then $LiAlH_4$. Then mix in the "dry" plastic (Kraton)
- After work with dry box is complete, place weighing dish in beaker with used paper towels before removing from dry box. Rinse disposables with water prior to disposal.
- Remove mixture of solids from the dry box and bring into the fume hood.

7.1.3 Adding the liquids:

- Mix in mineral oil plasticizer. Use the syringe.
- Add the solvent (toluene) last. Keep adding solvent until a homogeneous slurry is formed. This may require several times the amounts listed in the recipe worksheet. Wear a respirator with a charcoal filter while using toluene.

7.1.4 Evaporation:

- Evaporate under vacuum at room temperature. The vacuum pump must also be in the fume hood so that the toluene vapor is vented out of the lab.
- Check the pump every 5 or 10 minutes or so (to insure the pressure remains low enough to encourage evaporation). The mixture takes several hours to completely evaporate. Evaporation may be interrupted by placing the mixture inside an airtight jar (label the jar appropriately), and storing in the flammables cabinet overnight.

Evaporation is complete when the material consists of hardened chunks of material . It is helpful to stir the mixture if the dry surface is shielding undried mixture beneath the surface.

7.1.5 Pulverizing

- Use a blender with special attachment to pulverize mix down to a powder form. Mix on low power level and in short pulses (to prevent temperature rise). Occasionally touch the underside of the container to check the temperature.
- Pulverization is complete when grain size is the same throughout the mixture
- Store this powder inside airtight cans or jars

Analytic Power Corporation
C081
Recipe.wk4 to calculate weights of materials for hydrogen generator
Ref 68 - Analytic Power Bibliog.

Batch		10.00	gm (active)		Materials	Mwt.	T decomp
XS Hydride		200%	0-25% wt		NH4Cl	57.49	340
Stoich.		0.06	moles NH4CL		MgH2	26.33	280
Finished		11.40	gm (total)		CaH2	42.1	600
	gm moles		gm		NaBH4	37.83	420
NH4CL	0.0584		3.36		NaAlH4	53.96	?
LiAlH4	0.1751		6.64		LiBH4	21.78	273
					LiAlH4	37.95	125
XS Complex Hydride			0%	5-10% wt	Heat of RX	-3.322	kcal
	gm moles	mol H2	gm			kcal	kcal/gm
NaBH4	0.00	0.00	0.00			-3.32	-0.29
CaH2	0.00	0.00	0.00			-3.32	-0.29
LiBH4	0.00	0.00	0.00			-3.32	-0.29
LiAlH4	0.00	0.00	0.00			-3.32	-0.29

			gm		Hydrogen Yield	
Binder	10%	wt	1.00	Krayton (Shell SEBS)	0.41	gmmol
Plasticizer	30%	wt	0.30	Mineral Oil (Plasticizer)	0.80	liter/gm
Solvent	20%	wt plastic	0.10	Toluene (solvent)	0.80	liter/gm

7.2 Pellet Pressing

Analytic Power constructed a four-piece pellet mold that can press pellets 1 inch in diameter and up to four inches long. We also had a four-piece pellet mold that was built under a prior contract. This mold can press pellets 0.625 in. in diameter and 0.5 in. long. To press pellets with these molds first weigh the powder mixture. Calculate the required amount from the size of the pellet to be made (this may be measured from the pellet mold) and the desired pellet density (20 g/cu. in) the necessary amount of powder. For example, the small mold needs about 2.5 - 2.7 grams of powder for the formation of a pellet.

Place the bridgewire in the pellet by pressing the powder around the wire. The best results were found by placing Nickel Chromium wire in the center of the pellet (i.e., the center of the circular cross section, thus the wire length is in the axial direction of the cylindrical pellet). Three different sizes of Nickel Chromium wire were used: 32 gauge (0.0080 inch), 28 gauge (0.0126 inch), and 24 gauge (0.0201 inch). The 32 gauge wire is extremely thin and easily broken. The 24 gauge wire so large that it gets caught in the mold holes. The 28

gauge wire appears to be the best. It is very important not to break the wire during pressing. Continuity may be tested with an ohmeter.

Press the pellet to 3000 psi, if the small pellet mold is being used. Use 6500 psi for the larger mold, because the pellet has a larger diameter. Pressing the powder decreases the initial volume of the powder by half.

Log the details of the pellet used: which mixture batch is used, what is the wire thickness, pellet length, pellet diameter, pellet mass, and anything else that may appear relevant.

7.3 Recommended Redesign of the Pellet Mold

One of the challenges in forming pellets is pressing the powder around the wire while keeping the wire taut. If one end of the wire is attached to the bottom (stationary) platen and the other is attached to the (movable) male part that is adjacent to the press, the wire ends will be pushed together. This forces the middle of the wire to the side and yields poor ignition. A better way to press pellets is to hold the wire taut with a clamp that fits through a vertical slit inside the base of the movable male part, and is attached to the stationary bottom platen. This is shown in Figure 11.

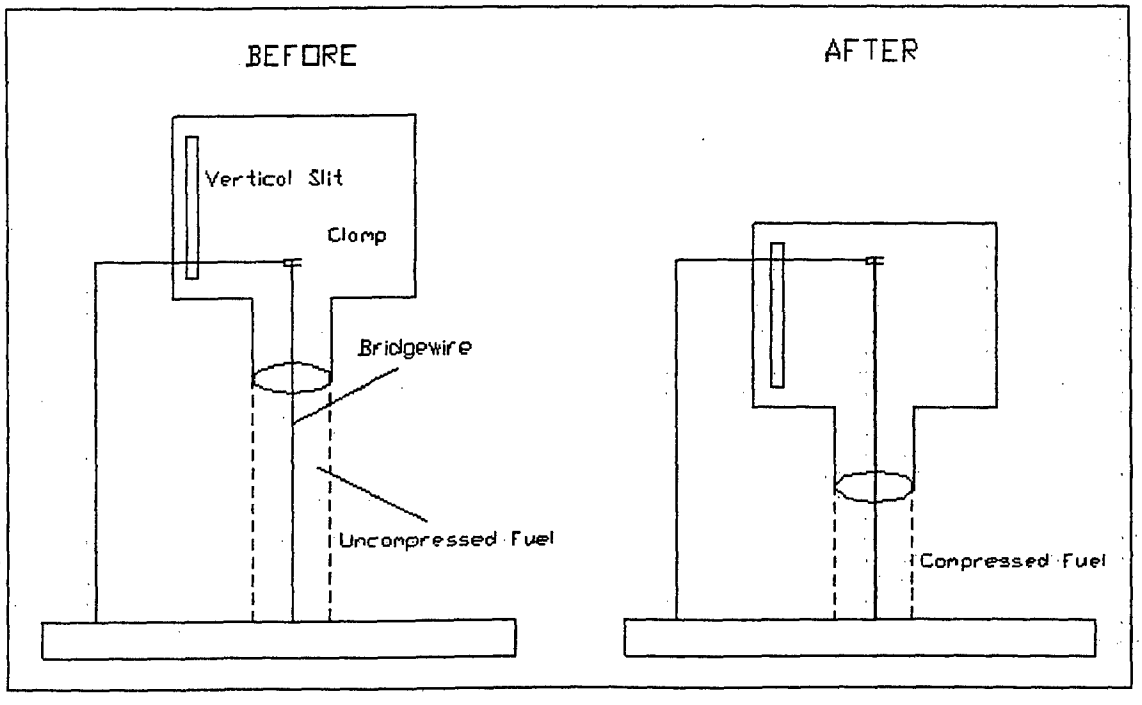

Figure 11: Sketch of Proposed Improved Mold Design

INPUT POWER PLANT DATA	HIT <CR> TO SELECT DEFAULT VALUE
NET POWER	150 WATTS, INPUT UPDATE?
INVERTER EFFICIENCY	100 %, INPUT UPDATE?
MECHANICAL EFFICIENCY	90 %, INPUT UPDATE?
SYSTEM PRESSURE	1.05 ATM, INPUT UPDATE?
CELL VOLTS	.7 , INPUT UPDATE?
AIR UTILIZATION	50 % , INPUT UPDATE?
HYDROGEN UTILIZATION	99.9 % , INPUT UPDATE?
CELL TEMPERATURE	130 degF , INPUT UPDATE?

HIT ANY KEY TO CONTINUE

CHEMICAL HYDRIDE PLANT PERFORMANCE DATA

OVERALL EFFICIENCY	50.4 %		
POWER:			
NET	165.8	watts	
GROSS	166.7	watts	
FUEL CELL	166.7	watts	
PARASITE	0.8	watts	
UTILIZATION:			
HYDROGEN	0.999		
OXYGEN	0.500		
TEMPERATURE:			
ANODE INLET	70.0	deg F	
CATHODE INLET	80.6	deg F	
CELL EXIT	130.0	deg F	

CELL		
CURRENT DENSITY	144.7	asf
CELL VOLTAGE	0.700	volts
OPEN CIRCUIT (dH/nF)	1.057	volts
CELL AREA	1646.0	ft2
ENERGY IN	1.1E+03	BTU/HR
AIR IN=	1.1E+03	BTU/HR
ENERGY FROM REACTION=	1.6E+02	BTU/HR
ENERGY OUT=	1.2E+03	BTU/HR
AIR OUT=	1.2E+03	BTU/HR
HYDROGEN OUT=	3.9E+01	BTU/HR

HIT ANY KEY TO CONTINUE

02-18-1997 13:59:47C069-1

MICROFLO NODE ARRAY

MOLAR FLOW RATES - lb mole/hr

NODE	1	4	5	7	8	9	10	11	12	13	14	15
H2	0.010	0.010	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
H2O	0.000	0.000	0.000	0.000	0.000	0.010	0.000	0.000	0.000	0.000	0.000	0.000
CH4	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
CO	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
CO2	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
O2	0.000	0.000	0.000	0.010	0.010	0.005	0.217	0.217	0.217	0.060	0.060	0.060
N2	0.000	0.000	0.000	0.037	0.037	0.037	0.817	0.817	0.817	0.227	0.227	0.227
NH3	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
TOTAL	0.010	0.010	0.000	0.047	0.047	0.052	1.034	1.034	1.034	0.288	0.288	0.288
T DEG F	130	130	130	70	81	130	70	70	130	70	70	130
P ATM	1.000	1.000	1.000	1.000	1.050	1.050	1.000	1.000	1.000	1.000	1.000	1.000
H BTU/HR	3.933E+01	3.933E+01	3.933E-02	1.737E+02	1.772E+02	-7.867E+02	3.842E+03	3.842E+03	4.275E+03	1.070E+03	1.070E+03	1.191E+03
S BTU/HR F	4.205E-01	4.205E-01	4.205E-04	2.082E+00	2.084E+00	2.399E+00	4.606E+01	4.606E+01	4.684E+01	1.283E+01	1.283E+01	1.305E+01
CP B/HR F	6.758E-02	6.758E-02	6.758E-05	3.255E-01	3.256E-01	3.704E-01	7.200E+00	7.200E+00	7.213E+00	2.006E+00	2.006E+00	2.009E+00

INPUT POWER PLANT DATA	HIT <CR> TO SELECT DEFAULT VALUE
NET POWER	150 WATTS, INPUT UPDATE?
INVERTER EFFICIENCY	100 %, INPUT UPDATE?
MECHANICAL EFFICIENCY	90 %, INPUT UPDATE?
SYSTEM PRESSURE	1.05 ATM, INPUT UPDATE?
CELL VOLTS	.7 , INPUT UPDATE?
AIR UTILIZATION	50 % , INPUT UPDATE?
HYDROGEN UTILIZATION	99.9 % , INPUT UPDATE?
CELL TEMPERATURE	130 degF , INPUT UPDATE?

HIT ANY KEY TO CONTINUE

CHEMICAL HYDRIDE PLANT PERFORMANCE DATA

OVERALL EFFICIENCY	50.4 %	CELL	
		CURRENT DENSITY	144.7 asf
POWER:		CELL VOLTAGE	0.700 volts
NET	165.8 watts	OPEN CIRCUIT (dH/nF)	1.057 volts
GROSS	166.7 watts	CELL AREA	1646.0 ft2
FUEL CELL	166.7 watts		
PARASITE	0.8 watts	ENERGY IN	1.1E+03BTU/HR
		AIR IN=	1.1E+03BTU/HR
		ENERGY FROM REACTION=	1.6E+02BTU/HR
UTILIZATION:			
HYDROGEN	0.999	ENERGY OUT=	1.2E+03BTU/HR
OXYGEN	0.500	AIR OUT=	1.2E+03BTU/HR
		HYDROGEN OUT=	3.9E+01BTU/HR
TEMPERATURE:			
ANODE INLET	70.0 deg F		
CATHODE INLET	80.6 deg F		
CELL EXIT	130.0 deg F		

HIT ANY KEY TO CONTINUE

02-18-1997 13:59:47C069-1

MICROFLO NODE ARRAY

MOLAR FLOW RATES - lb mole/hr

NODE	1	4	5	7	8	9	10	11	12	13	14	15
H2	0.010	0.010	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
H2O	0.000	0.000	0.000	0.000	0.000	0.010	0.000	0.000	0.000	0.000	0.000	0.000
CH4	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
CO	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
CO2	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
O2	0.000	0.000	0.000	0.010	0.010	0.005	0.217	0.217	0.217	0.060	0.060	0.060
N2	0.000	0.000	0.000	0.037	0.037	0.037	0.817	0.817	0.817	0.227	0.227	0.227
NH3	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
TOTAL	0.010	0.010	0.000	0.047	0.047	0.052	1.034	1.034	1.034	0.288	0.288	0.288
T DEG F	130	130	130	70	81	130	70	70	130	70	70	130
P ATM	1.000	1.000	1.000	1.000	1.050	1.050	1.000	1.000	1.000	1.000	1.000	1.000
H BTU/HR	3.933E+01	3.933E+01	3.933E-02	1.737E+02	1.772E+02	-7.867E+02	3.842E+03	3.842E+03	4.275E+03	1.070E+03	1.070E+03	1.191E+03
S BTU/HR F	4.205E-01	4.205E-01	4.205E-04	2.082E+00	2.084E+00	2.399E+00	4.606E+01	4.606E+01	4.684E+01	1.283E+01	1.283E+01	1.305E+01
CP B/HR F	6.758E-02	6.758E-02	6.758E-05	3.255E-01	3.256E-01	3.704E-01	7.200E+00	7.200E+00	7.213E+00	2.006E+00	2.006E+00	2.009E+00